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From: Wambaugh, John
Sent: Wed 7/31/2013 2:45:46 PM
Subject: RTK Oral Equivalent Doses
vLiverPBPK_0.8.tar.gz
evaluation-073113.pdf
RDynamic_0.8.tar.gz

Hi Everyone,

If you install the attached two R packages you should be able to have access to all RTK data by R function calls. I have added additional capabality to predict our own values (see the pretty decent comparison plot, also attached). The new functionality lets us use new data, estimate quantiles not used in the paper, and extrapolate to species beyond rat and human.

Keith -- if possible, I'd like to present this at next week's ToxCast meeting.

Please don't share this outside of the center yet. I will be working with Barbara Wetmore and a few others to try to publish the evaluation of this package this fall.

The following example calls should walk you through most of the relevant cases:

```
library(vLiverPBPK)

#Steady-state concentration (uM) for 1 mg/kg/day for 0.95 quantile for human for Acetochlor (published value):
Wetmore_Css(chem.CAS="34256-82-1")
#Steady-state concentration (uM) for 1 mg/kg/day for 0.95 quantile for human for Acetochlor (calculated value):
calc_vLiver_Css(chem.CAS="34256-82-1")
#Steady-state concentration (uM) for 1 mg/kg/day for 0.95 quantile for rat for Acetochlor (no published value, 0.5 quantile only):
Wetmore_Css(chem.CAS="34256-82-1",species="Rat")
```

#Steady-state concentration (uM) for 1 mg/kg/day for 0.95 quantile for rat for Acetochlor (calculated value):
calc_vLiver_Css(chem.CAS="34256-82-1",species="Rat")
#Steady-state concentration (uM) for 1 mg/kg/day for 0.5 quantile for rat for Acetochlor (published value):
Wetmore_Css(chem.CAS="34256-82-1",species="Rat",which.quantile=0.5)
#Steady-state concentration (uM) for 1 mg/kg/day for 0.5 quantile for rat for Acetochlor (calculated value):
calc_vLiver_Css(chem.CAS="34256-82-1",species="Rat",which.quantile=0.5)
#Steady-state concentration (uM) for 1 mg/kg/day for 0.95 quantile for mouse for Acetochlor (no published value, human and rat only):
Wetmore_Css(chem.CAS="34256-82-1",species="Mouse")
#Steady-state concentration (uM) for 1 mg/kg/day for 0.95 quantile for mouse for Acetochlor (calculated value):
calc_vLiver_Css(chem.CAS="34256-82-1",species="Mouse")

#State-state oral equivalent dose (mg/kg BW/day) to produce 0.1 uM serum concentration for human, 0.95 quantile, for Acetochlor (published value):
Wetmore_Oral_Equiv(0.1,chem.CAS="34256-82-1")
#State-state oral equivalent dose (mg/kg BW/day) to produce 0.1 uM serum concentration for human, 0.95 quantile, for Acetochlor (calculated value):
calc_vLiver_Oral_Equiv(0.1,chem.CAS="34256-82-1")
#State-state oral equivalent dose (mg/kg BW/day) to produce 0.1 uM serum concentration for human, 0.05, 0.5, and 0.95 quantile, for Acetochlor (published values):
Wetmore_Oral_Equiv(0.1,chem.CAS="34256-82-1",which.quantile=c(0.05,0.5,0.95))
#State-state oral equivalent dose (mg/kg BW/day) to produce 0.1 uM serum concentration for human, 0.05, 0.5, and 0.95 quantiles, for Acetochlor (calculated value):
calc_vLiver_Oral_Equiv(0.1,chem.CAS="34256-82-1",which.quantile=c(0.05,0.5,0.95))
#State-state oral equivalent dose (mg/kg BW/day) to produce 0.1 uM serum concentration for rat, 0.95 quantile, for Acetochlor (calculated value):
calc_vLiver_Oral_Equiv(0.1,chem.CAS="34256-82-1",species="Rat")
#State-state oral equivalent dose (mg/kg BW/day) to produce 0.1 uM serum concentration for mouse, 0.95 quantile, for Acetochlor (calculated value):
calc_vLiver_Oral_Equiv(0.1,chem.CAS="34256-82-1",species="Mouse")

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